Liouville's theorem for pedants

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January 8, 2015

Abstract

We discuss Liouville's theorem on the evolution of an ensemble of classical particles, using language friendly to differential geometers.

Contents

1 Liouville's theorem, classical statement

The classical statement of Liouville's theorem [4] is that an 'ensemble' of particles described by a density function $\rho = \rho(q_i, p_i, t)$ evolves in time according to the equation:

$$\frac{\partial \rho}{\partial t} + \sum_i \left(\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = 0,$$

where q_i, p_i are generalised coordinates on phase space and t is time. This note discusses its statement in modern language and tries to clarify the question to which Liouville's theorem is the answer.

2 Classical mechanics

Recall that the modern model of classical mechanics is a symplectic manifold (M, ω) together with a function:

$$H : M \to \mathbb{R},$$

the Hamiltonian.

This data determine a vector field X_H on M, the dual of dH under identification of TM and T^*M using ω. The defining equation is thus:

$$dH = i_{X_H}\omega,$$

where $i_{X_H}\omega = \omega(X_H, \cdot)$ is the interior product. X_H is known as the Hamiltonian vector field associated to H.

We obtain time evolution for the system (M, ω, H) by integrating X_H to its flow. I.e., the 1-parameter group of diffeomorphims[1]:

$$\phi : M \times \mathbb{R} \to M,$$

which generates X_H, constitutes time evolution. In other words, the integral curves of X_H represent physical motion according to H.

3 Liouville's theorem, modern statements

Consider the following:

Proposition 3.1. *Let (M, ω) be a symplectic manifold and X a vector field on M, then the following are equivalent:*

- *X is locally Hamiltonian.*
- $\mathcal{L}_X\omega = 0$.
- *The flow $\phi_t = \phi(\cdot, t)$ associated to X consists of symplectomorphisms.*

where $\mathcal{L}$ is the Lie derivative.

Proof. This follows easily from two characteristic properties of the Lie derivative, namely $\mathcal{L}_X = di_X + i_X d$ (together with the Poincaré lemma) as well as $\mathcal{L}_X = \lim\limits_{h\to 0}\left(\frac{\phi_h^* - id}{h}\right)$ (use $\frac{d}{dt}\phi_t^* = \phi_t^*\mathcal{L}_X$ to deduce $\phi_t^*\omega$ is constant). $\square$

[1] Technically ϕ may only be locally defined, i.e., it is a sheaf. We will not emphasise this since we would gain nothing by it here.

For some people, a modern statement of Liouville's theorem is:

Corollary 3.2. *If (M, ω, H) is a physical system then $\mathcal{L}_{X_H}\omega = 0$.*

Although the result is definitely relevant, it is somewhat distant from the classical statement: there is no sight of anything playing the role of ρ.

Others view a modern version of Liouville's theorem to be:

Corollary 3.3. *If (M, ω, H) is a physical system then ϕ_t consists of symplectomorphisms.*

A popular view [1, 3] is to regard the following slightly weaker result as the content of Liouville's theorem:

Corollary 3.4. *If (M, ω, H) is a $2n$-dimensional physical system then ϕ_t preserves ω^n, i.e., time evolution preserves volume in phase space.*

It's mostly just a matter of taste but my preference is to reserve Liouville's name for a proposition that mentions ρ and includes his equation.

Consider then a physical system about whose initial state we have incomplete information. Instead of our usual model of initial data as a distinguished point of phase space, we generalise and model initial data as a probability measure $\rho_0\omega^n$ on phase space for some function:

$$\rho_0 : M \to \mathbb{R},$$

which represents our information (and satisfies $\int_M \rho_0\omega^n = 1$).

Consider time evolution for ρ_0. Because classical mechanics is perfectly deterministic, the probability density $\rho(x, t)$ of a state $x \in M$ at any time t is uniquely determined: just follow the curve representing physical motion through x back for t units of time, reaching a point x_0, say. We must have:

$$\rho(x, t) = \rho_0(x_0).$$

In other words *prescribing the likelihood of an initial state is the same as prescribing the likelihood of the full history of physical motion through that state.* Let's capture this in a definition:

Definition 3.5. *Let (M, ω, H) be a physical system and let $\rho : M \times \mathbb{R} \to \mathbb{R}$. We say ρ obeys Newton's laws if $t \mapsto \rho(\alpha(t), t)$ is constant for all integral curves α of X_H.*

Note that a tautological restatement of the condition on ρ in definition 3.5 is:

$$\phi_t^*\rho_t = \rho_0 \qquad \text{for all } t,$$

where $\rho_t = \rho(\cdot, t)$ and as usual ϕ_t is the flow generating X_H. We can thus generalise corollary 3.4 as:

Proposition 3.6. *Let (M, ω, H) be a $2n$-dimensional physical system with flow ϕ_t and let $\rho : M \times \mathbb{R} \to \mathbb{R}$. Then ρ obeys Newton's laws iff*

$$\phi_t^* \mu_t = \mu_0 \qquad \text{for all } t,$$

where $\mu_t = \rho(\cdot, t)\omega^n$ is the probability measure on M at time t.

This means that classical mechanics remains measure-preserving, even when considering ensembles of particles. I suspect this important observation is the reason for the popularity of regarding corollary 3.4 as a modern statement of Liouville's theorem. I prefer to regard Liouville's theorem as the below answer to the question: which functions ρ obey Newton's laws?

Proposition 3.7. *Let (M, ω, H) be a physical system and let $\rho : M \times \mathbb{R} \to \mathbb{R}$. Then ρ obeys Newton's laws iff*

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0, \tag{1}$$

where $\{\cdot, \cdot\}$ is the Poisson bracket of (M, ω).

Proof. Differentiate $t \mapsto \rho(\alpha(t), t)$, use Hamilton's equations and require that the result be 0. ☐

There is one final point, due to Gibbs [2] worth mentioning: we can regard Liouville's differential equation (1) as a physical *continuity equation* for probability density flowing through phase space like a fluid with velocity X_H, and without sinks or sources.

The classical continuity equation for a fluid with density ρ and velocity vector field v expresses the local conservation of mass and is usually written:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0. \tag{2}$$

This can be seen to be analogous to (1) because a symplectic manifold carries a natural differential operator analogous to the Riemannian divergence operator appearing in (2).

Indeed a symplectic manifold carries a natural symplectic star operator:

$$\star : \wedge^k \simeq \wedge^{2n-k},$$

defined in exactly the same way as the better-known Hodge star operator from metric geometry. We also have the formal adjoint (wrt ω) of the exterior derivative:

$$d^* = (-1)^k \star d \star : \Omega^{k+1} \to \Omega^k.$$

Many of the properties familiar from metric geometry still hold (e.g., $d^{*2} = 0$) but a little linear algebra reveals an important difference between the symplectic and Hodge stars: the would-be symplectic 'Laplacian' vanishes[2], i.e., d and d^* anti-commute. In particular $d^*df = 0$ for any function f. It follows that we can express the Poisson bracket as:

$$\{f, g\} = d^*(fdg),$$

for any functions f, g. The operator d^* is symplectic divergence.

We thus have Gibbs's statement of Liouville's theorem in modern language:

Proposition 3.8. *Let (M, ω, H) be a physical system and let $\rho : M \times \mathbb{R} \to \mathbb{R}$. Then ρ obeys Newton's laws iff*

$$\frac{\partial \rho}{\partial t} + d^*(\rho dH) = 0.$$

4 Boundary conditions

The form of Liouville's equation appearing in proposition (3.8) is especially convenient for considering boundary conditions. Indeed, since the total probability density must be constant in time, any boundary condition for ρ must guarantee that it satisfies[3]:

$$0 = \frac{\partial}{\partial t} \int_M \star\rho = \int_M \star \frac{\partial \rho}{\partial t} = -\int_M d(\star \rho dH) = -\int_{\partial M} \star \rho dH \tag{3}$$

An important class of boundary conditions are those defined in terms of a smooth involution $\beta : \partial M \to \partial M$ such that:

$$\beta^*(\star dH) = \epsilon(\beta) \star dH \tag{4}$$

where:

$$\epsilon(\beta) = \begin{cases} 1 & \text{if } \beta \text{ is orientation reversing} \\ -1 & \text{if } \beta \text{ is orientation preserving} \end{cases}$$

Given such additional data β, the boundary condition is then:

$$\beta^* \rho = \rho \quad \text{on } \partial M, \tag{5}$$

[2]It is nevertheless still possible to do 'Hodge theory' on a symplectic manifold, see [5].
[3]The symplectic star operator satisfies $\star^2 = 1$ and the volume form is $\star 1$.

from which (3) follows trivially.

This class includes both the 'bounce back' and 'specular reflection' boundary conditions for a particle in a box[4].

Note that since M carries a natural trivialisation of $\wedge^{2n}T^*M$, the wedge product provides a natural isomorphism: $\wedge^{2n-1}T^*M \simeq (\wedge^1 T^*M)^* \simeq TM$, under which $\star dH$ corresponds to the Hamiltonian vector field X_H.

References

[1] V. I. Arnol′d. *Mathematical methods of classical mechanics*, volume 60 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1991. Translated from the 1974 Russian original by K. Vogtmann and A. Weinstein, Corrected reprint of the second (1989) edition.

[2] Josiah Willard Gibbs. On the fundamental formula of statistical mechanics, with applications to astronomy and thermodynamics. *Proceedings of the American Association for the Advancement of Science*, 33:57–58, 1884.

[3] L. D. Landau and E. M. Lifshitz. *Course of theoretical physics. Vol. 1*. Pergamon Press, Oxford-New York-Toronto, Ont., third edition, 1976. Mechanics, Translated from the Russian by J. B. Skyes and J. S. Bell.

[4] Joseph Liouville. Sur la théorie de la variation des constantes arbitraires. *J. Math. Pures Appl.*, 3:342–349, 1838.

[5] Li-Sheng Tseng and Shing-Tung Yau. Cohomology and Hodge theory on symplectic manifolds: I. *J. Differential Geom.*, 91(3):383–416, 2012.

[4] If $V \subset \mathbb{R}^n$ is the box and q_i are coordinates on $\mathbb{R}^n$ so that $(p_i, q_i) \mapsto \Sigma p_i dq_i$ are coordinates on $M = T^*V$, then bounce back fixes the q_i and sends $p_i \mapsto -p_i$ whereas specular reflection reverses only the component of p normal to ∂V.